

SC1 - Short Course #1

Simul and PeakMaster: freeware tools for understanding electromigration separations and method development

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<http://web.natur.cuni.cz/gas/index.html>

Electrophoresis, unlike chromatography, allows a more precise look into the mechanism of separation because its environment is much simpler than in chromatography; instead of the heterogeneous two phases in chromatographic systems, electrophoresis works in a homogeneous liquid solution of electrolytes. We have managed to implement the mathematical model of electromigration into two user friendly software tools, which describe the real behaviour quite well and greatly facilitate method development of electrophoretic separations.

The dynamical simulation software **Simul** solves nonlinear continuity equations numerically, which enables visualizing the distribution of any constituent of the particular separation system in the separation channel at any time. This way it gives a complete picture of the particular separation run. It allows inspection of stacking or sweeping phenomena, sharpening of zone edges, focusing of ampholytes in isoelectric focusing systems, etc.

The **PeakMaster** series of software is based on the linear theory of eigenmobilities. This concept allows prediction of some theoretical characteristics of the separated analytes, which are connected with the experimentally important quantities in the separation system. They are, e.g., pH, number, positions and shapes of system peaks, extent of electromigration dispersion, simulation of the electropherogram, separation in chiral environment.

This way the experimental trial-and-error approach in method development is replaced by the efficient and reliable computer simulation.